CMS Papers 2008

Pekka Pyykkö [1]
Department of Chemistry, University of Helsinki,
P.O.B. 55 (A.I. Virtasen aukio 1), FIN–00014 Helsinki, Finland

[1] *FAX: 358-9-191 50169, E-mail: Pekka.Pyykko@helsinki.fi.*

Preface

The present report will contain a cumulative record of papers, published by the Finnish Centre of Excellence in Computational Molecular Science ('CMS'). During the third year of operation (2008), all papers of the participant groups are included.

Pekka Pyykkö
Chairman, 2006-08

Bibliography

[1] Kluth P., Schnohr C.S., Pakarinen O.H., Djurabekova F., Sprouster D.J., Giulian R., Ridgway M.C., Byrne A.P., Trautmann C., Cookson D.J., Nordlund K. and Toulemonde M. (2008). Fine structure in swift heavy ion tracks in amorphous SiO_2. *Phys. Rev. Lett.*, **101**, 175503.

[2] Nordlund K., Järvi T.T., Meinander K. and Samela J. (2008). Cluster ion-solid interactions from meV to MeV energies. *Appl. Phys. A*, **91**(4), 561, invited paper.

[3] Vörtler K., Björkas C., Terentyev D., Malerba L. and Nordlund K. (2008). The effect of Cr concentration on radiation damage in Fe-Cr alloys. *J. Nucl. Mater.*, **382**, 24–30.

[4] Järvi T.T., Kuronen A., Hakala M., Nordlund K., van Duin A.C.T., W. A. Goddard I. and Jacob T. (2008). Development of a ReaxFF description for gold. *Eur. Phys. J. B.*, **66**, 75–79.

[5] Järvi T.T., Pakarinen J.A., Kuronen A. and Nordlund K. (2008). Enhanced sputtering from nanoparticles and thin films: Size effects. *Europhys. Lett.*, **82**, 26002.

[6] Holmström E., Kuronen A. and Nordlund K. (2008). Threshold defect production in silicon determined by density functional theory molecular dynamics simulations. *Phys. Rev. B*, **78**(4), 045202.

[7] Sun L., Krasheninnikov A.V., Ahlgren T., Nordlund K. and Banhart F. (2008). Plastic deformation of single nanometer-sized crystals. *Phys. Rev. Lett.*, **101**, 156101, see also commentary on article by S. Suresh and J. Li, Nature 456 (2008) 717.

[8] Samela J. and Nordlund K. (2008). Atomistic simulation of the transition from atomistic to macroscopic cratering. *Phys. Rev. Lett.*, **101**, 027601, and cover of issue 2. Also selected to Virtual Journal of Nanoscale Science & Technology Vol. 18 Issue 3 (2008).

[9] Djurabekova F. and Nordlund K. (2008). Atomistic simulation of the interface structure of Si nanocrystals embedded into amorphous silica. *Phys. Rev. B*, **77**, 115325, also selected to Virtual Journal of Nanoscale Science & Technology Vol. 17 Issue 13 (2008).

[10] Djurabekova F., Backman M. and Nordlund K. (2008). Atomistic modelling of the interface of Si nanocrystal structures in a-SiO2 before and after ion irradiation. *Nucl. Instr. Meth. Phys. Res. B*, **266**, 2683.

[11] Gan Y., Kotakoski J., Krasheninnikov A.V., Nordlund K. and Banhart F. (2008). The diffusion of interstitial atoms in carbon nanotubes. *New J. Phys.*, **10**, 023022.

[12] Samela J., Nordlund K., Popok V.N. and Campbell E.E.B. (2008). Origin of complex impact craters on native oxide coated silicon surfaces. *Phys. Rev. B*, **77**, 075309, this also has the description of the Samela-Watanabe potential.

[13] Djurabekova F., Björkas C. and Nordlund K. (2008). Atomistic modelling of the interface structure of Si nanocrystals in silica. *J. Phys.: Conf. Ser.*, **100**, 052023.

[14] Nordlund K. and Dudarev S.L. (2008). Interatomic potentials for simulating radiation damage effects in metals. *Comptes Rendus Physique*, **9**(3-4), 343–352.

[15] Träskelin P., Saresoja O. and Nordlund K. (2008). Molecular dynamics simulations of C_2, C_2H C_2H_2, C_2H_3, C_2H_4, C_2H_5, C_2H_6 bombardment of diamond (111) surfaces. *J. Nucl. Mater.*, **375**(2), 270.

[16] Juslin N. and Nordlund K. (2008). Pair potential for Fe-He. *J. Nucl. Mater.*, **382**(2-3), 143–146.

[17] Negi S., Warrier M., Chaturvedi S. and Nordlund K. (2008). Molecular dynamics simulation of carbon nanotubes interacting with a graphite surface. *Journal of Computational and Theoretical Nanoscience*, **5**, 348353.

[18] Björkas C., Nordlund K., Malerba L., Terentyev D. and Olsson P. (2008). Simulation of displacement cascades in $Fe_{90}Cr_{10}$ using a two band model potential. *J. Nucl. Mater.*, **372**, 312–317.

[19] Keinonen J., Djurabekova F., Nordlund K. and Lieb K.P. (2008). Light Emitting Defects in Ion-Irradiated Alpha-Quartz. In *Silicon nanophotonics: Basic Principles, Present Status and Perspectives*, (Edited by Khriachtchev L.), chap. 14, pp. 379–396, World Scientific, Singapore.

[20] A V Krasheninnikov (2008). Atomistic Computer Simulations of Irradiation-Induced Effects in Nanostructured Carbon Materials. *Journal of Computational and Theoretical Nanoscience*, **5**, 1828–1851.

[21] V Skakalova and A B Kaiser and U Dettlaff and K Arstila and A V Krasheninnikov and J Keinonen and S Roth (2008). Electrical properties of C^{4+} irradiated single-walled carbon nanotube paper. *Physica Status Solidi B-Basic Solid State Physics*, **245**, 2280–2283.

[22] Jusélius J. and Sundholm D. (2008). Polycyclic antiaromatic hydrocarbons. *Physical Chemistry Chemical Physics*, **10**(44), 6630–6634.

[23] Lehtonen O., Sundholm D. and Vänska T. (2008). Computational studies of semiconductor quantum dots. *Physical Chemistry Chemical Physics*, **10**(31), 4535–4550.

[24] Robert Send and Dage Sundholm (2008). The molecular structure of a curl-shaped retinal isomer. *Journal of Molecular Modeling*, **14**(8), 717–726.

[25] Olli Lehtonen and Dage Sundholm (2008). Computational studies of free-standing silicon nanoclusters. In *Silicon Nanophotonics: Basic Principles, Present Status and Perspectives*, (Edited by L Khriachtchev), chap. 3, pp. 61–88, World Scientific, Singapore.

[26] de Macedo L.G.M. and Pyykkö P. (2008). Bonding trends in M=CH_2 systems: Simple orbital interpretation and evidence for double bonds. *Chem. Phys. Lett.*, **462**, 138–143.

[27] Bieroń J., Froese Fischer C., Jönsson P. and Pyykkö P. (2008). Comment on the magnetic dipole hyperfine interaction in the gold atom ground state. *J. Phys. B*, **41**, 115002.

[28] Pyykkö P. and Zaleski-Ejgierd P. (2008). From nanostrips to nanorings: the elastic properties of gold-glued polyauronaphthyridines and polyacenes. *Phys. Chem. Chem. Phys.*, **10**, 114–120.

[29] Pyykkö P. and Zaleski-Ejgierd P. (2008). Basis-set limit of the aurophilic attraction using the MP2 method: The examples of $[ClAuPH_3]_2$ dimer and $[P(AuPH_3)_4]^+$ ion. *J. Chem. Phys.*, **128**, 124309.

[30] Pyykkö P. (2008). Theoretical chemistry of gold. III. *Chem. Soc. Rev.*, **37**, 1967–1997.

[31] Pyykkö P. (2008). Year-2008 nuclear quadrupole moments. *Mol. Phys.*, **106**, 1965–1974.

[32] Riedel S., Kaupp M. and Pyykkö P. (2008). Quantum chemical study of trivalent Group 12 fluorides. *Inorg. Chem.*, **47**, 3379–3383.

[33] Karttunen A.J., Linnolahti M., Pakkanen T.A. and Pyykkö P. (2008). Icosahedral Au_{72}: a predicted chiral and spherically aromatic golden fullerene. *Chem. Comm.*, pp. 465–467, electronically published 15 November 2007.

[34] Zaleski-Ejgierd P., Patzschke M. and Pyykkö P. (2008). Structure and bonding of the MCN molecules, M=Cu, Ag, Au, Rg. *J. Chem. Phys.*, **128**, 224303.

[35] Pyykkö P. and Elmi F. (2008). Deuteron quadrupole coupling in benzene: Librational corrections using a temperature-dependent Einstein model and summary. The symmetries of electric field gradients and conditions for $\eta = 1$. *Phys. Chem. Chem. Phys.*, **10**, 3867–3871.

[36] Riedel S., Straka M. and Pyykkö P. (2008). Theoretical mapping of new L-(N^+)-L family of species with donor-acceptor bonding between N^+ and ligand. *J. Mol. Str. (THEOCHEM)*, **860**, 128–136.

[37] Sumerin V., Schulz F., Atsumi M., Wang C., Nieger M., Leskelä M., Repo T., Pyykkö P. and Rieger B. (2008). Molecular tweezers for hydrogen: Synthesis, characterization, and reactivity. *J. Am. Chem. Soc.*, **130**, 14117–14119.

[38] Weijo V., Manninen P. and Vaara J. (2008). Effect of molecular size on the parity-non-conserving contributions to the nuclear magnetic resonance shielding constant. *Theoretical Chemistry Accounts*, **121**, 53.

[39] Straka M., Lantto P. and Vaara J. (2008). Toward calculations of the ^{129}Xe chemical shift in Xe@C_{60} at experimental conditions: Relativity, correlation, and dynamics. *Journal of Physical Chemistry A*, **112**, 2658.

[40] Taubert S., Straka M., Pennanen T.O., Sundholm D. and Vaara J. (2008). Dynamics and magnetic resonance properties of Sc_3C_2@C_{80} and its monoanion. *Physical Chemistry Chemical Physics*, **10**, 7158.

[41] Pennanen T.O. and Vaara J. (2008). Nuclear magnetic resonance chemical shift in an arbitrary electronic spin state. *Physical Review Letters*, **100**.

[42] Riedel S., Straka M. and Pyykkö P. (2008). Theoretical mapping of new L-(N+)-L family of species with a donor-acceptor bonding between N+ and ligand L. *Journal of Molecular Structure: THEOCHEM*, **860**, 128.

[43] Telenius J., Wallin A.E., Straka M., Zhang H., Mancini E.J. and Tuma: R. (2008). RNA packaging motor: From structure to quantum mechanical modelling and sequential-stochastic mechanism. *Computational & Mathematical Methods in Medicine*, **9**, 351.

[44] Taubert S., Sundholm D., Juselius J., Klopper W. and Fliegl H. (2008). Calculation of magnetically induced currents in hydrocarbon nanorings. *Journal of Physical Chemistry A*, **112**, 13584.

[45] Ikäläinen S., Lantto P., Manninen P. and Vaara J. (2008). Laser-induced nuclear magnetic resonance splitting in hydrocarbons. *Journal of Chemical Physics*, **129**.

[46] Johansson M.P., Vaara J. and Sundholm D. (2008). Exploring the stability of golden fullerenes. *Journal of Physical Chemistry C*, **112**, 19311.

[47] Tanskanen H., Khriachtchev L., Lignell A., Räsänen M., Johansson S., Khyzhniy I. and Savchenko E. (2008). Formation of noble-gas hydrides and decay of solvated protons revisited: Diffusion-controlled reactions and hydrogen atom losses in solid noble gases. *Physical Chemistry Chemical Physics*, **10**(5), 692–701.

[48] Andersson T., Sumela M., Khriachtchev L., Räsänen M., Aseyev V. and Tenhu H. (2008). Solution properties of an aqueous poly(methacryl oxyethyl trimethylammonium chloride) and its poly(oxyethylene) grafted analogue. *Journal of Polymer Science B: Polymer Physics*, **46**(6), 547–557.

[49] Bochenkova A.V., Khriachtchev L., Lignell A., Räsänen M., Lignell H., Granovsky A.A. and Nemukhin A.V. (2008). Hindered rotation of HArF in solid argon: Infrared spectroscopy and a theoretical model. *Physical Review B*, **77**(9), 094301.

[50] Novikov S., Sinkkonen J., Nikitin T., Khriachtchev L., Räsänen M. and Haimi E. (2008). Free-standing SiO2 films containing Si nanocrystals directly suitable for transmission electron microscopy. *Microelectronics Journal*, **39**(3-4), 518–522.

[51] Khriachtchev L., Isokoski K., Cohen A., Räsänen M. and Gerber R.B. (2008). A small neutral molecule with two noble-gas atoms: HXeOXeH. *Journal of the American Chemical Society*, **130**(19), 6114–6118.

[52] Khriachtchev L. (2008). Rotational isomers of small molecules in noble-gas solids: From monomers to hydrogen-bonded complexes. *Journal of Molecular Structure*, **880**(1-3), 14–22.

[53] Lehtinen O., Sun L., Nikitin T., Krasheninnikov A.V., Khriachtchev L., Rodrguez-Manzo J.A., Terrones M., Banhart F. and Keinonen J. (2008). Ion irradiation of carbon nanotubes encapsulating cobalt crystals. *Physica E*, **40**, 2618–2621.

[54] Lignell A., Lundell J., Khriachtchev L. and Räsänen M. (2008). Experimental and computational study of HXeY–HX complexes (X, Y = Cl and Br): An example of exceptionally large complexation effect. *Journal of Physical Chemistry A*, **112**(24), 5486–5494.

[55] Likonen J., Vainonen-Ahlgren E., Khriachtchev L., Coad J.P., Rubel M., Renvall T., Arstila K. and Hole D.E. (2008). Structural investigation of re-deposited layers in JET. *Journal of Nuclear Materials*, **377**(3), 486–491.

[56] Lignell A. and Khriachtchev L. (2008). Intermolecular interactions involving noble-gas hydrides: Where the blue shift of vibrational frequency is a normal effect. *Journal of Molecular Structure*, **889**(1-3), 1–11.

[57] Khriachtchev L., Nikitin T., Oton C.J., Velagapudi R., Sainio J., Lahtinen J. and Novikov S. (2008). Optical properties of silicon nanocrystals in silica: Results from spectral filtering effect, m-line technique, and X-ray photoelectron spectroscopy. *Journal of Applied Physics*, **104**(10), 104316.

[58] Leonid Khriachtchev (2008). Silicon Nanocrystals in Silica: Optical Properties and Laser-Induced Thermal Effects. In *Silicon Nanophotonics: Basic Principles, Present Status and Perspectives*, (Edited by L Khriachtchev), chap. 11, pp. 297–325, World Scientific, Singapore.

[59] L Khriachtchev, (Ed.) (2008). *Silicon Nanophotonics: Basic Principles, Present Status and Perspectives*. World Scientific, Singapore.

[60] Räsänen M. (2008). Physical Chemistry – Cool it, baby. *Nature*, **453**(7197), 862–863.

[61] Seetula J. and Eskola A. (2008). Kinetics of the R + HBr RH + Br (CH_3CHBr, $CHBr_2$ or $CDBr_2$) equilibrium. Thermochemistry of the CH_3CHBr and $CHBr_2$ radicals. *Chemical Physics*, **351**(1-3).

[62] A J Eskola and R S Timonen and P Marshall and E N Chesnokov and N Evgeni and L N Krasnoperov (2008). Rate constants and hydrogen isotope substitution effects in the CH_3+HCl and CH_3+Cl_2 reactions. *Journal of Physical Chemistry A*, **112**(32), 7391–7401.

[63] A J Eskola and I Golonka and M P Rissanen and R S Timonen (2008). Kinetics of the CCl_2+Br_2 and CCl_2+NO_2 reactions in the temperature range 266-365 K and reactivity of the CCl_2 biradical. *Chemical Physics Letters*, **460**(4–6), 401–405.

[64] Garden A.L., Halonen L. and Kjaergaard H.G. (2008). Calculated Band Profiles of the OH-Stretching Transitions in Water Dimer. *The Journal of Physical Chemistry A*, **112**(32), 7439–7447.

[65] Vainio M., Peltola J., Persijn S., FJM F.J.M.H. and Halonen L. (2008). Singly resonant cw OPO with simple wavelength tuning. *Optics Express*, **16**(15), 11141–11146.

[66] Hänninen V., Garden A.L., Kjaergaard H.G., Tennyson J. and Halonen L. (2008). Calculation of the O-H stretching vibrational overtone spectrum of the water dimer. *Journal of Physical Chemistry A*, **112**(28), 6305–6312.

[67] Pesonen J. (2008). Kinetic energy operators in linearized internal coordinates. *The Journal of Chemical Physics*, **128**(4), 044319.